

PETSc on GPU: Available Preconditioners and Performance Comparison with CPU

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1 Introduction

PETSc (short for Portable Extensible Toolkit for Scientific Computation) is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations (PDEs). It is free for everyone including industrial users (see [BBB⁺11]) and very well supported (compare [BBB⁺10]). PETSc is written in ANSI-C and usable from C, C++, FORTRAN 77/90 and Python. It employs the MPI standard and is thus portable to any system supporting MPI.

PETSc is developed as open-source which makes any kind of modifications and extensions possible. Hence PETSc is used by a vast number of scientific applications and software packages. Furthermore, the open development process of PETSc has facilitated the formation of a large and active community. Not least because of its community PETSc supports all major external scientific software packages (Matlab, Mathematica, FFTW, SuperLU, ...) making it possible to call e.g. Matlab in a PETSc code.

The current stable version of PETSc (3.1, released March 25, 2010) comes with data structures for sequential and parallel matrices and vectors, sequential and parallel time-stepping solvers for ordinary differential equations, direct linear solvers, iterative linear solvers (many Krylov subspace methods) with preconditioners and nonlinear solvers. In the current development version of PETSc support for NVIDIA GPUs via the CUDA library has been added. The purpose of this work was to test the performance and usability of PETSc on up to date NVIDIA GPUs.

2 Using PETSc

Although PETSc is written in C it works with objects. These objects are hierarchically organized which (ideally) makes it obsolete for the user to interact directly with C-primitives or storage duration specifiers. Figure 2.1 illustrates the hierarchical organization of PETSc. An immediate consequence of the use of abstraction layers is that

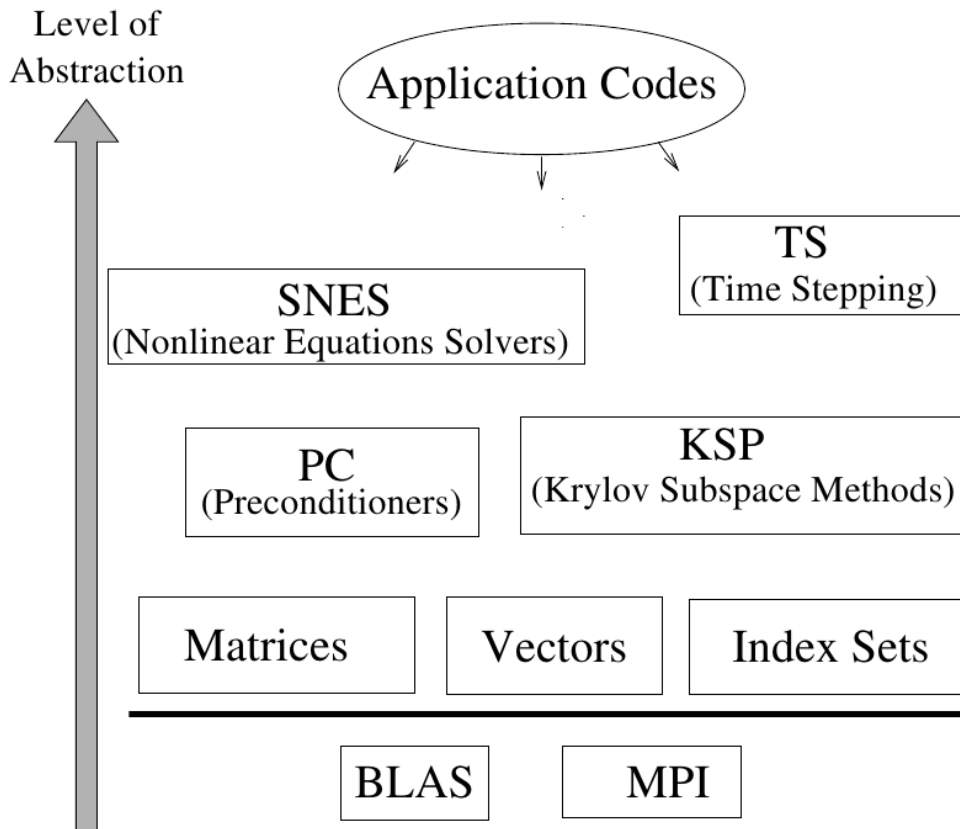


Figure 2.1: Organizational diagram of the PETSc libraries. Taken from [BBB⁺10].

data is propagated "bottom up", i.e. top-level abstraction objects (like PDE-solvers) do not access data in the underlying C-array directly but use methods on PETSc-vector and -matrix objects. Hence if all low-level PETSc-objects are ported to CUDA all high-level abstraction objects run on the GPU without any code modification. Following this idea the current development version of PETSc introduces new vector and matrix implementations whose methods run entirely on the GPU using CUDA. In the following the basic steps for setting up PETSc and using its new GPU support are explained.

2.1 Installation

A note of caution at the beginning: the installation procedure laid out here was tested and is intended for a specific version of PETSc operated on specific hardware. This is by no means meant to be a tutorial on how to set up PETSc in general. For readers looking for such a tutorial the PETSc-homepage [BBB⁺11] is the place to go.

As mentioned above the GPU support of PETSc is realized by implementing new vector and matrix objects in CUDA. This implementation is done by using the CUDA

libraries Thrust [HB10] and Cusp [BG10]. Since at the time this text was written Thrust, Cusp and PETSc were still under development it was necessary to obtain the newest Cusp/Thrust versions from NVIDIA mercurial repositories in order to build the newest PETSc development version. However, since this work was carried out in the course of a PhD-seminar on GPU-computing the intention was to install PETSc on a server reserved for seminar participants who were simultaneously pursuing other CUDA-programming projects, many of them relying on Cusp/Thrust. Therefore constantly updating Cusp/Thrust seemed to be impractical and potentially jeopardous for the stability of other projects. Hence the latest PETSc version compatible to the already installed Cusp/Thrust libraries was chosen, namely version 15257:a0abdf539b1e from November 3rd, 2010.

The following installation procedure refers to the "fermi"-server (IP: 143.50.47.245) equipped with two GeForce GTX 480 on an ASUS P6T Deluxe V2 mainboard powered by an Intel Core i7-920 CPU and 6GB Corsair XMS3 DIMM RAM running Ubuntu Linux 10.04.2 LTS 64bit. In the following we denote by the environmental variable `PETSC_DIR` the full path to the PETSc home directory (for a local PETSc-installation on a *nix system this is probably something like `$HOME/petsc_dev/`) while `PETSC_ARCH` specifies the local architecture and compiler options (by using different `PETSC_ARCH` one can handle different sets of libraries). The versions of CUDA, Cusp and Thrust needed by PETSc are listed in `PETSC_DIR/config/PETSc/packages/cuda.py`. Assuming that all NVIDIA software is properly installed and `nvcc` is in the path one has ensure that `LD_LIBRARY_PATH` points to the CUDA libraries (in our case using the `bash`: `LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/cuda/lib64`) then `export LD_LIBRARY_PATH`). Then PETSc is configured by issuing the following command in the `PETSC_DIR`-directory:

```
./config/configure.py --with-debugging=1 --with-cuda=1 --with-cusp=1
--with-thrust=1 --with-mpi-dir=/usr/lib/openmpi --with-c2html=0
```

The meaning of the `configure`-options is given below:

`with-debugging=1` compiles PETSc with debugging support (default). For performance runs this should be turned off but for developing code it is highly recommended to let it turned on (compare [BBB⁺10]).

`with-cuda=1` compiles PETSc with CUDA support. This option is currently only available in development versions of PETSc. It checks whether compatible NVIDIA kernel developer drivers are installed and all necessary binaries are in the path.

`with-thrust=1` looks for Thrust in default locations (usually `/usr/local/cuda/`). If Thrust is not installed in its default place the option `--with-thrust-dir=/path/to/thrust` may be used. This option is currently only available in development versions of PETSc.

`with-cusp=1` looks for Cusp in default locations (usually `/usr/local/cuda/`). If Cusp is not installed in its default place the option `--with-cusp-dir=/path/to/cusp`

may be used. This option is currently only available in development versions of PETSc.

`with-mpi-dir=/usr/lib/openmpi` points to the system's MPI installation. The user manual [BBB⁺10] claims that PETSc looks for MPI in all known standard locations. Even so it did not find the openMPI installation on fermi though the location cannot be called "exotic". However, this can as well be a problem of the development-version that may be fixed in future stable releases.

`with-c2html=0` prevents PETSc from using the optional package `c2html` for its documentation (used since `c2html` was not installed on fermi).

Note that if the GPU of the computer PETSc should be built on supports only single precision arithmetic (not the case with fermi's two GeForce GTX 480) the option `--with-precision=single` has to be given as well. It is further assumed that the system has a valid BLAS/LAPACK installation in default locations (otherwise the option `--with-blas-lapack-dir=/path/to/libs` has to be used). If BLAS/LAPACK is not yet installed the option `--download-f-blas-lapack=1` may be used to download and build a local BLAS/LAPACK installation (the same can be done with MPI using `--download-mpich=1`). However, due to performance reasons a system-wide installation of MPI/BLAS/LAPACK should be preferred.

After successful completion of the `configure`-stage PETSc is built by

```
make all
```

The source code of PETSc has more than 80 MB, so building may take a while. When the building is done the standard, i.e. non-CUDA, libraries can be tested by

```
make test
```

At present the only way to test the CUDA-functionality of PETSc is to build and run a tutorial example for the nonlinear solvers:

```
cd PETSC_DIR/src/snes/examples/tutorials
make ex19
./ex19 -da_vec_type mpicuda -da_mat_type mpiailcuda -pc_type none
-dmmg_nlevels 1 -da_grid_x 100 -da_grid_y 100 -log_summary -mat_no_inode
-preload off -cuda_synchronize
```

If both tests complete successfully PETSc can use NVIDIA GPUs.

2.2 Writing PETSc Code

Again a note of caution at the beginning: this section is *not* a programming guide. The purpose of the following is to give the reader a first glimpse of how PETSc-programs are written. Please refer to the user manual [BBB⁺10] for a comprehensive guide to PETSc programming and consult the website [BBB⁺11] for numerous tutorial examples. Since the author has written his code in C what follows refers to using PETSc from C. Note that though all PETSc routines are accessible in the same way no matter if the user's code is written in C/C++, FORTRAN 77/90 or Python there are language specific differences (e.g. FORTRAN starts indexing with 1, C/C++ and Python use zero-based indexing)

that have to be taken into account. Further details can be found on the PETSc-homepage [BBB⁺11].

Shown here is the exemplary use of PETSc to solve the linear equation system $Ax = b$, where $A \in \mathbb{R}^{N \times N}$ is some regular matrix and x and b are vectors in \mathbb{R}^N . In order to use PETSc from C the correct header has to be used, in our case

```
#include "petscksp.h"
```

which automatically includes all necessary low-level objects (PETSc-matrices, -vectors, ...). As laid out above PETSc's abstraction-layer design (and consequently its CUDA-features) can only be exploited adequately if the user's code is designed to solely use PETSc-specific data structures. Hence we do not use standard C variables but initialize the following PETSc-objects:

```
Mat A;                                (the coefficient matrix A as PETSc-matrix)
Vec x, b;                             (the solution x and the right hand side b as PETSc-vectors)
KSP ksp;                              (a linear solver object)
PetscInt N;                           (the dimension of the linear system as PETSc-integer)
```

Usually before anything else there should be the call

```
PetscInitialize(&argc,&argv,(char *)0,help);
```

which initializes the PETSc database and calls `MPI_Init()`. Note that `PetscInitialize()` has to be called before any PETSc-related function is used. Next the coefficient matrix is created:

```
MatCreate(PETSC_COMM_WORLD,&A);
```

Every PETSc-object supports a basic interface (`Create()`, `Get/SetName()`, `Get/SetType()`, `Destroy()`,...) similar to class methods in C++ (hence the `Create()` routine can be seen as an equivalent to a C++ constructor). Therefore everything in this section is only discussed for PETSc-matrices but works analogously for PETSc-vectors (where it makes sense) only with the prefix `Vec` instead of `Mat` in the corresponding calls. Note that `PETSC_COMM_WORLD` is the PETSc-version of `MPI_COMM_WORLD` (for details see [BBB⁺10]). The size of the matrix has to be determined by

```
MatSetSizes(A,PETSC_DECIDE,PETSC_DECIDE,N,N);
```

By using `PETSC_DECIDE` the portions of the matrix held by each processor are determined by PETSc (assuming that `A` is a parallel PETSc-matrix). The next call is one of the most powerful features of PETSc: by using the method `SetFromOptions()` the implementation type of a PETSc-object can be set at runtime using command line options (if no options are given default values are used). Hence by calling

```
MatSetFromOptions(A);
```

the type of the PETSc-matrix `A` is either assumed to be parallel sparse on the CPU (default) or it can be set by using the following command line options:

```
-mat_type aij sequential/parallel (depending on the number of MPI-processes) sparse
matrix on the CPU
```

```
-mat_type seqdense sequential dense matrix on the CPU
```

```
-mat_type mpdense parallel dense matrix on the CPU
```

-mat_type seqbaij sequential block sparse matrix on the CPU

-mat_type mpibaij parallel block sparse matrix on the CPU

-mat_type aijcuda sequential/parallel (depending on the number of MPI-processes) sparse matrix on the GPU

Note that currently only sequential/parallel sparse matrices, i.e. no block or dense types, are supported on the GPU. For performance reasons any (large) matrix should be pre-allocated before values are inserted. Assuming the PETSc-matrix **A** is parallel the call

```
MatMPIAIJSetPreallocation(A,...);
```

allocates memory for **A** given the number of nonzeros per diagonal and off-diagonal portion of **A** (see [BBB⁺10] for actual function arguments and further details). Once memory has been allocated

```
MatSetValues(A,...);
```

inserts entries into the matrix **A**. Note that in this stage the matrix is not yet ready to use since `MatSetValues()` generally caches the matrix entries. Therefore it is necessary to call

```
MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
```

```
MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);
```

to finally assemble the matrix. Next the solver object can be created:

```
KSPCreate(PETSC_COMM_WORLD,&ksp);
```

The call

```
KSPSetOperators(ksp,A,A,SAME_NONZERO_PATTERN);
```

tells the solver that **A** is the system matrix (here the matrix that defines the linear system also serves as preconditioner). Like PETSc-matrices and -vectors any PETSc-solver object has a `SetFromOptions()` method, namely

```
KSPSetFromOptions(ksp);
```

which either defines the solver to be a GMRES method with block Jacobi preconditioner (default) or sets its attributes at runtime using the command line options `-ksp_type <solver>` and `-pc_type <preconditioner>` (for a comprehensive list of available solvers and preconditioners as well as the many other adjustable options of PETSc-solvers, please refer to [BBB⁺10]). Having defined all necessary components of the linear system $Ax = b$ in PETSc we can now solve it:

```
KSPSolve(ksp,b,x);
```

The solution **x** can be examined or saved using the `View()` method of the PETSc-vector **x**. When PETSc-objects are no longer needed they should be freed. In our case by

```
VecDestroy(x); VecDestroy(b); MatDestroy(A); KSPDestroy(ksp);
```

which is (analogously to the `Create()` method) equivalent to a C++ destructor. At the end of every PETSc-program the call

```
PetscFinalize();
```

ensures the proper termination of the PETSc database and all MPI processes.

Note that all PETSc routines are passing references (to avoid unnecessary copies of variables) and return a PETSc-specific error code. Therefore it is strongly recommended to always call PETSc routines using PETSc's error code (which was omitted above only

for the sake of brevity). The error code is also a PETSc variable that has to be declared properly:

```
PetscErrorCode ierr;
```

Then a typical function call is for instance

```
ierr = MatCreate(PETSC_COMM_WORLD,&A);CHKERRQ(ierr);
```

where `CHKERRQ(ierr)` checks the error code, calls the appropriate handler and returns (propagates errors from bottom up). This makes debugging of PETSc codes much easier.

Note further that it is of course possible to hard-code the implementation type of an object, i.e. the use of the `SetFromOptions()`-method is not stringently required. If for instance a matrix has to be a parallel MPI matrix for a program to work properly one should prefer to explicitly write

```
ierr = MatSetType(A,MATMPIAIJ);CHKERRQ(ierr);
```

in the code over using `MatSetFromOptions()` in combination with the command line argument `-mat_type mpiai`. However, when running PETSc programs on NVIDIA GPUs the `SetFromOptions()`-method should be employed in any case since debugging on the GPU is currently very difficult (compare [BBB⁺11]).

2.3 Building and Running PETSc Programs

The author wants to emphasize again that this section (just as the previous one) refers to using PETSc from C on a *nix-like system. If the reader wants to build PETSc code written in C++, FORTRAN 77/90 or Python please consult the manual [BBB⁺10].

Since an average PETSc code is linked to (literally) dozens of libraries the use of Makefiles to automate the building process becomes mandatory. In the simplest case of one source code file, namely `first_code.c`, a sample PETSc-Makefile is given below

```
PETSC_DIR = /home/user/petsc-3.1-p3

include ${PETSC_DIR}/conf/variables
include ${PETSC_DIR}/conf/rules

first_code: first_code.o chkopts ${CLINKER} -o first_code
            first_code.o ${PETSC_LIB} ${RM} first_code.o
```

Further information about Makefiles for PETSc codes can be found in the corresponding chapter of the manual [BBB⁺10]. The executable binary file `first_code` generated by the command `make first_code` (assuming the building process succeeded without errors) can be executed by

```
mpirun -np <n> ./first_code -petsc_option1 pvalue1 -petsc_option2 pvalue2
... -user_option1 uvalue1 -user_option2 uvalue2 ...
```

where `<n>` denotes the number of MPI processes. Note that any PETSc program can use its own options (denoted as `-user_option` above) together with PETSc's options. A list of all available PETSc-options can be either found in the manual [BBB⁺10] or by using `./first_code -help` (which can of course be combined with the classical C

statement `static char help = "help text";` in the source code `first_code.c`). Examples of C code illustrating the use of PETSc and user-defined options can be found online [BBB⁺11].

3 Numerical Results

This section presents the profiling results documenting the performance of PETSc version 15257:a0abdf539b1e on the fermi server. Note that since this work in progress version of PETSc was already outdated by the time this text was written the results shown here have to be seen as preliminary and do not reflect the final library performance.

3.1 Motivation: An Image Processing Problem

The following brief excursion to image processing is merely intended to provide a motivational problem that leads to a PDE which can be solved with PETSc. We consider an image denoising problem (the following derivation is mainly taken from [AK06, Chap. 3]). Let $\Omega := [1, N]^2 \subset \mathbb{R}^2$ with $N \in \mathbb{N}$ and $f, u : \Omega \rightarrow \mathbb{R}$. Assume that u is the unknown original image and f is the given degraded data (for the sake of simplicity we consider here only gray-scale images; otherwise u and f would not be scalar but vector valued). We want to recover u from f which is a so-called *image reconstruction problem*. Thus we first of all need a model linking u to f . One of the simplest and most widely used (compare [AK06, Chap. 3]) is the linear relation

$$f = u + \eta,$$

where η is a noise term. To solve this *inverse problem* we make some assumptions on η : suppose η is white Gaussian noise then according to the maximum likelihood principle the solution of the least squares problem

$$(3.1) \quad \inf_u \int_{\Omega} |f - u|^2 d\mathbf{x},$$

is an approximation to the original image. However, in this form $u \equiv f$ is the minimizer of (3.1). Thus we introduce a regularization term. We define the functional

$$(3.2) \quad J(u) := \frac{1}{2} \int_{\Omega} |f - u|^2 d\mathbf{x} + \frac{1}{2} \int_{\Omega} |\nabla u|^2 d\mathbf{x},$$

and consider the minimization problem

$$(3.3) \quad \min_{u \in H^1(\Omega)} J(u).$$

Note that for $u \in H^1(\Omega)$ and $f \in L^2(\Omega)$ problem (3.3) is well defined and admits a unique solution (see for instance [AK06, Chap. 3]). Thus the use of min instead of inf in (3.3) is justified. Note further that usually the second term enters the cost functional J with an additional (multiplicative) parameter λ . However, in practice choosing λ "correctly" is

not trivial. Hence for the sake of simplicity (but at the expense of the solution's quality) we relinquish the use of λ .

The first term in (3.2) measures the fidelity of u to the given data f while the second term (first introduced by Tikhonov and Arsenin [TA77] in 1977) penalizes oscillations in the gradient of u . This means that the minimizer of (3.2) is not only supposed to be close to the given data but also a solution with low gradient and hence low noise level is favored.

The classical approach to solve the minimization problem (3.3) is to use variational calculus: we compute the Gâteaux derivative of J in an arbitrary direction $v \in C^\infty(\bar{\Omega})$, i.e. we compute

$$\frac{\delta J}{\delta u}(u; v) := \left. \frac{d}{ds} J(u + sv) \right|_{s=0},$$

for some scalar parameter $s \in \mathbb{R}$. This yields

$$\begin{aligned} \left. \frac{d}{ds} J(u + sv) \right|_{s=0} &= \frac{d}{ds} \left(\frac{1}{2} \int_{\Omega} |f - (u + sv)|^2 d\mathbf{x} + \frac{1}{2} \int_{\Omega} |\nabla u + s \nabla v|^2 d\mathbf{x} \right) \Big|_{s=0} \\ &= \int_{\Omega} (f - u)v d\mathbf{x} + \int_{\Omega} \nabla u \cdot \nabla v d\mathbf{x} \\ &= \int_{\Omega} (f - u)v d\mathbf{x} + \int_{\partial\Omega} v \nabla u \cdot \mathbf{n} dS - \int_{\Omega} v \Delta u d\mathbf{x}, \end{aligned}$$

where we used partial integration to shift derivatives from v to u . The weak necessary optimality condition for the minimization of J is

$$\frac{\delta J}{\delta u}(u; v) = 0, \quad \forall v \in C^\infty(\bar{\Omega}).$$

Assuming that u is sufficiently regular we may apply the fundamental Lemma of calculus of variations to obtain

$$\begin{cases} \Delta u + u = f \text{ in } \Omega, \\ \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega, \end{cases}$$

the so-called *Euler–Lagrange equations* associated to the optimization problem (3.3). However, for the sake of notation in the numerical community we rewrite it into

$$(3.4) \quad \begin{cases} -\Delta u - u = -f \text{ in } \Omega, \\ \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega. \end{cases}$$

To solve the PDE (3.4) with PETSc we discretize it using central finite differences with a unit step size $h = 1$. Then the discrete version of the Laplacian operator with Neumann boundary conditions under lexicographic ordering is a large sparse block matrix:

$$-\Delta_h := \begin{pmatrix} B & -I & & & \\ -I & C & -I & & \\ & \ddots & \ddots & \ddots & \\ & & -I & C & -I \\ & & & -I & B \end{pmatrix} \in \mathbb{R}^{N^2 \times N^2},$$

with blocks

$$C := \begin{pmatrix} 3 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 3 \end{pmatrix} \in \mathbb{R}^{N \times N},$$

and

$$B := C - I_N,$$

where $I_N \in \mathbb{R}^{N \times N}$ is the identity matrix and N denotes the image dimension. Let $\vec{f} \in \mathbb{R}^{N^2}$ and $\vec{u} \in \mathbb{R}^{N^2}$ denote the discrete versions of the noisy image and the original image under lexicographic ordering respectively. Then the Euler–Lagrange equations (3.4) are discretized by

$$(3.5) \quad A\vec{u} = \vec{f},$$

where

$$A := -\Delta_h - I_{N^2}.$$

Note that it is well known that the Laplace operator has very strong smoothing properties and thus tends to blur edges [AK06]. Since the Laplacian in the Euler–Lagrange equation (3.4) arises from the L^2 -norm of the gradient of u in the corresponding weak formulation (3.2) the idea is to use the L^1 -norm in (3.2) instead. One of the first who followed this idea were Rudin, Osher and Fatemi in their ground breaking work [ROF92]. Using the L^1 -norm of ∇u , also called *total variation* of u , proved to be highly successful in practice. And when Chambolle published a projection algorithm [Cha04] the numerical solution of total variation based models could be realized in a computationally very efficient way. However, having in mind that the purpose of this work was to test PETSc’s performance on NVIDIA GPUs the use of total variation minimization together with Chambolle’s algorithm did not seem suitable since it does not involve the solution of linear systems. Thus we employed the above model leading to the PDE (3.4) although the approach is not state of the art (a novel approach that generalizes the total variation and overcomes some of its drawbacks is the so-called *total generalized variation* [BKP09]).

3.2 Performance Tests

We solve the discrete Euler–Lagrange equation (3.5) using PETSc and compare its performance on the CPU and on the GPU. All runs were carried out with PETSc version 15257:a0abdf539b1e on the fermi server described above. This PETSc version supports the following GPU features:

- two CUDA vector implementations: `seqcuda` and `mpicuda`
- two CUDA matrix implementations: `seqaijcuda` and `mpiaijcuda`

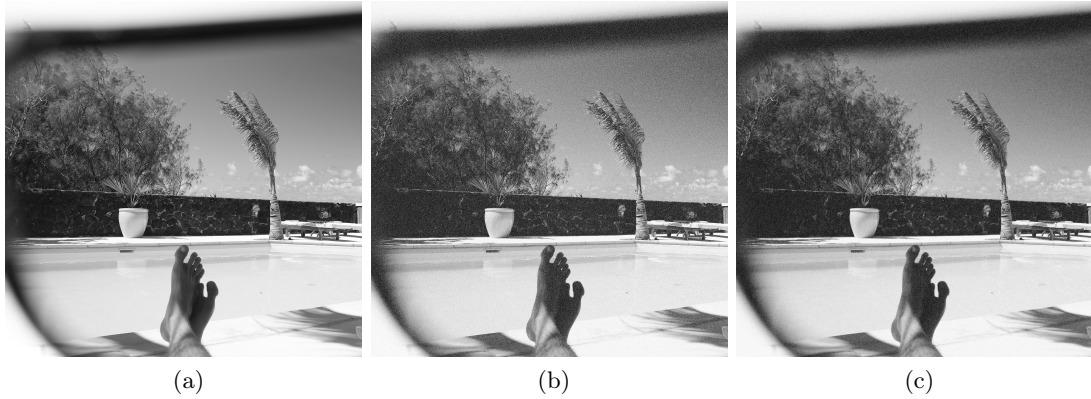


Figure 3.1: The original gray scale test image (a), the noisy image f (b) and the computed reconstruction u (c).

- all Krylov methods except `ibcgs` (an improved stabilized version of the bi-conjugate gradient squared method, see [YB02]) run on the GPU (`ibcgs` violates PETSc's hierarchical abstraction layer design by directly accessing data in the underlying C arrays; hence it needs to be rewritten to run on the GPU)
- the preconditioners `jacobi`, `bjacobi` (block Jacobi) and `asm` (an restricted additive Schwarz method, see [DW]) run on the GPU

Note that the discrete Laplacian Δ_h is a textbook example of a sparse block matrix that can be stored memory efficiently by exploiting its inherent symmetries and block structure. However, since the PETSc version used here only supports sequential or parallel sparse matrices on the GPU neither the block structure nor symmetries of Δ_h have been taken into account in the implementation of (3.5). Nevertheless, as indicated above PETSc provides matrix formats on the CPU which can utilize symmetry and block structure of a matrix. Even so, for better comparison to the GPU performance these formats have not been used.

The code for solving (3.5) was developed using the `SetFromOptions()` method. This way it was possible to run the same code both on the CPU and on the GPU using only different command line options. After finalization of the implementation process PETSc was recompiled using the `--with-debugging=0` option to obtain better performance in the test runs.

The original gray scale test image used here is depicted in Figure 3.1 (a). The noisy image f (depicted in Figure 3.1 (b)) was obtained by adding 35% Gaussian white noise to the original image. The image dimension was $N = 1290$ thus giving $N^2 = 1\,664\,100$ unknowns and 8315340 nonzero entries in the coefficient matrix A of (3.5).

The profiling results of the solution of (3.5) using PETSc for the given noisy image f are summarized in Table 1. The command line options used to obtain the CPU results were

CPU/GPU	Preconditioner	Iterations	Time (sec) (All/Solve/Copy)	Memory (MB)
PETSc-CPU	bjacobi	6	2.3/0.2/–	348
	jacobi	15	2.7/0.5/–	223
	asm	5	2.2/0.2/–	271
PETSc-GPU	bjacobi	6	1.9/0.1/0.05	304
	jacobi	15	1.7/0.1/0.01	268
	asm	5	2.1/0.1/0.1	242

Table 1: Profiling results of solving (3.5) using PETSc on the fermi server with two MPI processes. The first three rows show the CPU-performance of PETSc, the last three rows illustrate its GPU-performance. The default linear solver GMRES with standard options has been used. The second column indicates the employed preconditioners, the third column shows how many GMRES-iterations were needed to satisfy the default convergence criterion. The fourth column depicts the runtime (in seconds) of the whole program, the time needed to solve (3.5) and the time spent copying data from host to device and vice versa. Finally the rightmost column shows PETSc’s memory consumption (in Megabytes).

```
-mat_type mpiai j -vec_type mpi -pc_type jacobi/bjacobi/asm
-log_summary -memory_info
```

for the GPU results the options

```
-mat_type mpiaijcuda -vec_type mpicuda -pc_type jacobi/bjacobi/asm
-log_summary -memory_info
```

have been used. The computed solution u is depicted in Figure 3.1 (c). For better visual evaluation the upper right portion of the corrupted image f and the computed reconstruction u is given in Figure 3.2. Note that the computed image u still contains noise and suffers from blurred edges. These are known negative effects of employing the Laplacian for image denoising that can be reduced by either including a regularization parameter λ (as explained in the previous section) or by utilizing a more sophisticated cost functional, e.g. a total variation based cost. However, as stated above the purpose of this work was not to obtain a preferably well reconstructed image but to profile PETSc’s performance on the GPU.

The performance boost by running our code on the GPU using this version of PETSc was surprisingly small. It seems that the (preliminary) implementation of the preconditioners on the GPU is not memory efficient yet: when using the restricted additive Schwarz preconditioner **asm** copying data back and forth between host and device took approximately as long as solving the system (3.5). For the block Jacobi preconditioner **bjacobi** the copy-time summed up to 50% of the solution time. The most efficient preconditioner (referring to the copying time) was the Jacobi preconditioner in our profiling runs. However, note that these results have to be interpreted with caution: the PETSc mailing list confirms that newer versions of Cusp/Thrust/PETSc do not exhibit the same problems. But for reasons explained above these new versions could not be tested on

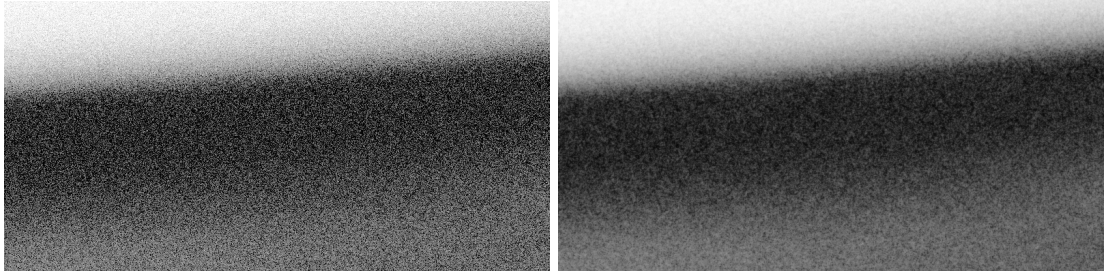


Figure 3.2: Image detail of the corrupted data f (left) and the computed reconstruction u (right).

fermi. Moreover, the memory consumption given in Table 1 seems to be inaccurate in this PETSc version either.

4 Conclusions

Summarized the CUDA capabilities of PETSc are extremely promising. People who are already using PETSc can "port" code to run on NVIDIA GPUs by using a simple command line option. For anyone not familiar with PETSc the way of doing GPU programming PETSc offers may be compelling for two reasons: first (and most important) due to PETSc's abstraction layers the user does not have to be concerned with GPU hardware details - PETSc hides away CUDA specifics in the GPU-vector and -matrix methods. Second the possibility to easily switch between CPU and GPU makes the development process very flexible: if in the course of code-writing the decision is made to test the application on the GPU it can be done with minimal amount of work (assuming the code is written solely using PETSc's datatypes). Hence in terms of CPU/GPU flexibility PETSc is currently unrivaled. However, these advantages have a price: mastering PETSc takes time. Though the user manual [BBB⁺10] is comprehensive and well structured it takes rather long (compared to classic C or Python at least) to write a first working PETSc-program. Thus PETSc is probably most attractive to people dealing with very complex large scale problems that demand high performance state of the art numerical methods. The newly included CUDA capabilities make PETSc competitive (and in some respect superior) to any other modern high performance computing software but are at this time probably not the decisive factor to port existing code to PETSc.

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